

35. VISUALIZING THE QUANTUM ATOM

Abstract: Students from the advanced high school classes up to the last university years have difficulties in grasping the notions involved in the description of the Quantum Atomic Model (QAM). Many researchers suggest that using Information and Communication Technologies (ICT) for visualizing the QAM would improve students' understanding. An empirical study was conducted with 20 first-year students of the Department of Primary Education. They interacted with two Internet-based software packages, considered as representative 3D visualizations of the QAM. For the analysis of our results, a qualitative approach was taken by using SOLO (Structure of the Observed Learning Outcomes) taxonomy. Our results indicated that software packages concerning the 3D representations of QAM do not help students to understand scientific concepts and the atomic shape. The article proposes the use of Virtual Reality Technologies for the creation of atomic visualizations based on scientific data that support conceptual change

Keywords: 3D visualization, Information and Communication Technologies, Quantum Atomic Model, SOLO taxonomy

1. INTRODUCTION

It is generally accepted that Quantum Mechanics has a mysterious and exciting flavour because it deviates markedly from intuitive expectations and the 'normalcy' of the classical world. Yet, this strange theory is remarkably successful at describing the behaviour of real physical systems.

The structure of matter is a fundamental topic in science education from primary school up to the university level. It is well documented that students at all levels have conceptual difficulties in understanding the concepts associated with the particle nature of matter and mostly with the atomic models (Harrison and Treagust, 2000; Taber, 2003).

The Quantum Atomic Model (QAM) covers a part of the upper secondary and tertiary curriculum in many countries. As learning about the QAM involves a fundamental reconceptualization in many areas (Thacker et al., 2002), students from the advanced high school classes up to the last university years have difficulties in grasping the main notions. Students' misconceptions concern concepts such as the charge cloud, the probability of electron localization, indeterminacy, spin (Johnston et al., 1998; Budde et al., 2002a, b; Cassinelo and Gallego, 2005), as well as fundamental principles like the uncertainty principle (Müller and Wiesner, 1999; Budde et al., 2002a) or the law of quantum measurement (Johnston et al., 1998;

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Budde et al., 2002a) which are far from their intuition. It is also found that mechanical atomic models are dominating among secondary school and university students. These models are mostly taught in high school classes, they are more plausible, and their optical representations are concrete and comprehensible, so students recall them easily and even draw them without difficulty, since among other natural learning styles the visual-spatial is a prominent one (Barnea and Dori, 2000). Thus, many researchers propose visualization tools and suggest that using Information and Communication Technologies (ICT) for visualizing the QAM would improve students' understanding for three main reasons:

- It is complicated to create comprehensive three dimensional (3D) visual representations of the QAM without the advantage of ICT (Byrne, 1996; Barnea and Dori, 1999, 2000; Dori and Barak, 2001; Cataloglou and Robinett, 2002; Trindade et al., 2002; Barak, 2007).
- As the QAM is covered by a highly mathematical formalism and there is not yet consensus about how it might be taught less abstractly (Johnston et al., 1998), it can be described in a qualitative way taking advantage of ICT. Using the visualizations, students will be able to assimilate more abstract mathematical methods later in their careers (Byrne, 1996; Tuvi and Nachmias, 2001; Cataloglou and Robinett, 2002).
- The use of visualizations is an appropriate method for probing student understanding as many of them are not able to visualize the QAM in 3D space and to rotate the 3D model in their mind. Also, students lack depth perception and have limited sense of perspective when all they have seen are two dimensional (2D) representations or mathematical models (Hurwitz et al., 1999; Cataloglou and Robinett, 2002).

By the term 'visualization' we mean the optical hermeneutic transformation of scientific data and not the artistic rendering of a phenomenon. Visualization is the optical representation of information as the result of a simulation based on a scientific model.

The software packages referring to visualizations of the QAM which have been used as educational tools have the following characteristics: they are 2D or 3D visualizations based on simulations according to Quantum Atomic Theory and provide a certain level of interactivity. By rotating, for example, the 3D representations, students may become familiar with the shapes in space.

However,

- it is not often clarified if the wave function ψ , the probability density ψ^2 , or the electron density is represented through the 3D visualizations;
- the use of different colours for all these representations may create misconceptions;
- the nucleus position is not referred in relation to different representations;
- the difference between the hydrogen wave functions (orbitals) and the wave functions describing polyelectronic atoms is not explicitly mentioned;
- it is not made clear under which conditions the hydrogen orbitals, except 1s, describe the atom state.

Since quite a few reports describe the results of using these visualizations as educational tools, we investigate if they help students to understand the basic concepts involved in the construction of the QAM and create mental models in coherence with scientific knowledge.

The axes of our study are to investigate the following:

- How students conceive the 3D representations
- If students are able to connect the visualizations of wave functions with the basic principles of Quantum Theory
- Which are students' mental models for the atom after interacting with the visualizations
- If students prefer 3D representations and for what reason.

Here, a part of our research is presented concerning the visualization of the QAM using ICT. More specifically, the goal of our study is to propose dynamic 3D visualizations of the atom giving an integrated picture, avoiding misconceptions coming from the classical atomic models, as well as from the piecemeal presentation of ψ and ψ^2 or the lack of their comprehensive visualization.

2. METHODS AND SAMPLE

Since 1999 in upper secondary school the Greek chemistry courses have included the QAM, the atomic structure according to this model, as well as the explanation of covalent bonding based on valence bond theory without the use of any mathematical formalism. At the same grade, physics courses have included in chronological order all the atomic models which had been constructed before the development of Quantum Mechanics.

An empirical study was conducted in March 2004. Twenty first-year students of the Department of Primary Education, University of Ioannina, participated. These 17-year-old students have been taught the topics under study during their last year in high school, as described above.

Students interacted with two Internet-based software packages, considered as representative 3D visualizations of the QAM. First, it was 'Orbitron' that presents visualizations of atomic orbitals from 1s up to 7g. It includes representations of the wave function ψ , its radial distribution, electron density, and electron density with dots (Winter, 2002). Secondly, students used 'visualization of atomic orbitals using VRML' (Blauch, 2001). This involves representations of ψ radial distribution, electron density, and isosurface plots.

We chose these two packages as the most appropriate comparing with others found in the Web because by using them it is made clear which wave function is represented each time, and it is clarified if hydrogen orbitals or orbitals of a polyelectronic atom are represented and electron density plots and isosurface plots are included for every wave function.

After the interaction with the visualizations referred to hydrogen 1s, 2px, 2py, 2pz orbitals and electron density with dots ($e\psi^2$), each student participated in

a semi-structured interview. The most important sets of questions are presented below:

1. What these images represent? What kind of information do we get? Do they concern a certain chemical element? (we refer to 1s, 2px, 2py, 2pz orbitals visualizations). Describe how you conceive the notion of 'orbital'.
2. What these images represent? What kind of information do we get? Do they concern a certain chemical element? (we refer to 1s, 2px, 2py, 2pz electronic density plots with dots, which we call charge cloud as well). Describe how you conceive the notion of charge cloud.
3. Is it possible any of these images to represent an atom, if it were possible to see it somehow? Where it would be the nucleus?
4. According to uncertainty principle it is not possible to determine with accuracy the position and velocity of a particle. Why does it happen? Is there any relation between this principle and the images you have seen?
5. Do you prefer these 3D orbital representations than the 2D ones which are shown in your textbook?

Each one of the above sets consists of more than one question. This is because our aim was to make an in-depth analysis of the students' mental representations concerning the topic under study. For the analysis of our results, a qualitative approach was taken since we are interested in the exploration of cognitive content of students' answers by making an in-depth analysis of them. In the qualitative outlook, it is assumed that students learn cumulatively, interpreting and incorporating new material with what they already know, their understanding progressively changing as they learn (Biggs, 1994). Since knowledge is described with qualitative terms that focus on the cognitive content of students' answers, we use SOLO (Structure of the Observed Learning Outcomes) taxonomy for the data analysis (Biggs and Collis, 1982).

The SOLO taxonomy is an important application of cognitive theory to modern education. The SOLO taxonomy has evolved steadily since its initial formulation and now stands as a detailed model that can be used to explore and help in the interpretation of cognitive development in a range of learning areas. In so doing, it provides insights into the way understanding develops. This taxonomy provides five different levels of understanding, from prestructural to the deepest level, known as extended abstract. The reason we have chosen SOLO taxonomy is because we wanted to classify the students' answers into hierarchical levels and compare them with the scientific acceptable knowledge that is the extended abstract fifth level.

The SOLO taxonomy classifies students' understanding in the following five hierarchical levels.

Prestructural: Student is distracted or misled by irrelevant aspects. He avoids or repeats the question, makes an irrelevant association. In a transitional stage, he uses inadequately a relevant datum.

Unistructural: Student focuses on the relevant domain and works with a single aspect. He selects one relevant datum and closes on that. In a transitional stage, he selects two relevant but inconsistent data.

Multistructural: Student provides correct material with discrete, separate pieces of information that may be combined to provide a composite picture. He selects two or more relevant data, uses them inconsistently, and reaches an alternative conclusion. In a transitional stage, he recognizes inconsistencies but cannot resolve them.

Relational: Student offers an integrating understanding of the information. His answer has a coherent structure and meaning. He uses most or all relevant data, integrate them with a relating concept, and reaches a right conclusion. In a transitional stage, he tries to generalize his conclusion without success.

Extended abstract: Student provides abstract principles or hypotheses that show the specific example as just one of many possible results.

The 20 students' answers have been examined and analysed towards the following components for being evaluated and classified to a certain level:

- The recognition of characteristics for describing an atomic model according to a scientific theory.
- The correlation of the above elements in order to be consistent with the basic principles of the scientific theory according to which the atomic model is constructed.
- The deduction of a consistent conclusion for the representation of an atom according to the atomic model described above.

Transitional responses have been also detected that carry more information than usual in the level the student is emerging from, but he is not reaching at the next SOLO level.

3. DATA ANALYSIS AND RESULTS

Among the students' answers we have detected the first four SOLO levels and two transitional ones showing their development of understanding, after their interaction with the visualizations (Table 1).

More specifically, students' performance to each question is presented below.

Question set 1

Most of students' answers (17) reached up to the third SOLO level. They did not realize that the representations which they have seen were graphs of hydrogen ψ wave function at the ground state (1s orbital) or at the first excited state (2p orbitals).

TABLE 1. Students' SOLO Levels ($N = 20$)

| Solo levels | Question 1 | Question 2 | Question 3 | Question 4 |
|--------------------|------------|------------|------------|------------|
| 1. Prestructural | 2 | 6 | 16 | 18 |
| 2. Unistructural | 5 | 6 | 3 | 1 |
| 2→3 Transitional | 5 | 1 | 0 | 0 |
| 3. Multistructural | 5 | 3 | 0 | 1 |
| 3→4 Transitional | 3 | 3 | 0 | 0 |
| 4. Relational | 0 | 1 | 1 | 0 |

Answer example of the 2–3 transitional level:

x, y, z are the orbitals. 1s, 2p, 2s are subshells. The colour intensity shows the number of electrons. The orbitals' shapes are the same for all chemical elements. I don't remember what an orbital exactly is. Is it the space where the electrons move? No....

The student referred more than one characteristic concerning the orbital, but they are not all correct.

Five students, whose answers are categorized to the third level, recognized the graphs as orbitals, but they were not able to combine the information given by the picture with that they had learned about wave functions in order to differentiate the two atomic orbitals. They simply referred Schrödinger equation without connecting its solutions with the concept of the orbital.

Answer example of the multistructural level 3:

They are orbitals ... There are one 1s orbital and three 2p orbitals. There is the Schrödinger equation ... There is a probability to find out the electron somewhere. The orbitals are always the same for all the chemical elements.

The student referred different characteristics concerning the atomic orbitals, most of them correct, but she did not even try to combine them.

Three students whose answers reached the 3rd to 4th transitional level tried to explain the different schemes of atomic orbitals 1s and 2p, the correlation between orbitals and Schrödinger equation or the difference between the orbitals for hydrogen and polyelectronic atoms without success.

Answer example of the 3–4 transitional level:

I can see the 1s and 2p orbitals for hydrogen; they must be different for polyelectronic atoms ... I remember that Schrödinger equation gives us some information about orbitals, I can't remember which one. We have one 1s orbital but three 2p orbitals because for 1s: $n=1$ and $l=0$ (one value) and for 2p: $n=2$ and $l=-1, 0, 1$ (three values). I don't know why they have different representations.

The student referred different characteristics which are all correct. He also tried to relate them but he did not arrive to a correct conclusion about the information given by the 3D representations with which he had interacted before.

Question set 2

The students had great difficulty in describing what a charge cloud is, because it is not explicitly expressed in the Chemistry textbook. They confused the charge cloud with that of the orbital, as they have seen that both have the same contour. Consequently, 6 of the students are at the prestructural level and 16 did not attain further than the third level. There was only one answer at the relational level.

Answer example of the prestructural level 1:

They are orbitals. All these dots ... I don't know, we can only measure the force from the nucleus to hydrogen.

The student gave an irrelevant answer as he confused the concepts 'orbital' and 'charge cloud'.

Answer example of the relational level 4:

'They are charge clouds; the densest area of the cloud is where we have the bigger probability of finding the electron. But there is very small possibility for the electron to be found too far from the nucleus, that's why there are quite a few dots there'.

The student used all the relevant data correctly and reached to the correct conclusions, but she was not able to generalize so as to arrive at the formulation of the uncertainty principle.

Question set 3

Almost all of the students did not know neither if the orbitals' graphs represent the atom, nor the position of the nucleus. Only one gave an answer which is classified at the fourth (relational) level. This may have happened because the notions of ψ , ψ^2 , or electron density in their textbooks are not related with the shape of an atom at the ground or excited state.

Answer example of the unistructural level 2:

'These shapes must have some relation with the atom's shape, but I don't know exactly ... the nucleus is at the middle of them'.

The student referred only one relevant data. Except that she was not able to say something about the atom's shape.

Answer example of the relational level 4:

'In general the electron orbitals in the outer shells must determine the scheme of an atomic model. So the hydrogen atom must be spherical as the charge cloud which is determined by the 1s orbital. The nucleus is at the centre of the sphere'.

In this answer the information given by the optical representation was related with student's knowledge for arriving at a right conclusion about the atomic model. Therefore the student had conceived that all these 3D images concern the atomic models but he could not generalize about the scheme of an atomic model in the ground or in the excited state.

Question set 4

All the students seemed not to have assimilated the uncertainty principle. Only one student's answer categorized to the third level, while 19 answers considered being at the two first levels.

Answer example of the prestructural level 1:

'We can't measure the position and the velocity of an electron exactly'.

The student repeated the uncertainty principle without giving any other explanation.

Answer example of the multistructural level 3:

'It is applied to the electrons, because they move very fast, so a very precise instrument is required'.

The student related this principle with the microcosm, but she was not able to go deeper and face the electrons as quantum and not classical objects.

Concerning the fifth question set, 16 students preferred the 3D representations than the 2D shown in their textbooks. They experienced the different 3D graphs

concerning the structure of charge density and they understood better their shape in space. They also asked for more interactivity that might help them to comprehend the atom shape.

According to our findings, most of the students did not overcome the third level of SOLO taxonomy, while no one reached the fifth. They were able to refer some of the QAM characteristics, but they could not correlate them with the principles of Quantum Mechanics in order to come to a conclusion about the shape of the hydrogen atom and the properties of its electron.

4. CONCLUSIONS AND IMPLICATIONS

The aim of our study was to explore student's mental representations about the QAM. In particular, we tried to discover if the use of 3D graphics concerning atomic orbitals help them to describe the QAM and grasp the main notions involved in coherence with most important principles. The results of our study revealed that the students do not conceive:

- The concept of the orbital as the wave function ψ (or probability function of presence), which describes the state of an electron in an atom and not as 'a region in space inside which there is a given probability for the electron to be located'.
- The information given by the wave function ψ , the probability density ψ^2 , and the charge density concerning the atom state they describe.
- How the charge density is correlated with the notion of the charge cloud.
- The differences between the state function ψ for describing the hydrogen atom and the polyelectronic atoms in the ground state.
- How the energy level determines the shape of the charge cloud in space for the hydrogen atom and the polyelectronic ones.
- That the uncertainty principle is an inherent attribute in microcosm; it is the result of the wave-particle duality and the unavoidable interaction between the observed quantum object and the observing instrument.
- How the uncertainty principle is related with the charge cloud notion and the non-deterministic nature of microcosm according to Quantum Mechanics.
- Which is the shape of an atom in the ground state.
- How the shape of an atom is changed if this atom interacts with a photon and it 'moves' to an excited state.

Besides, the students did not mention the electron's wave nature as they supposed electrons to be particles that move very fast. So, in agreement with our results Johnston and his colleagues (1998), Petri and Niedderer (2001), Olsen (2002), Tsaparlis and Papafotis (2002) have found that students at the last class of high school or at university level describe electrons as classical particles.

Summarizing, our results indicated that the students confused the characteristics of planetary and QAM models even after having interacted with the visualizations. They also could not distinguish the two atomic models and figure

out their limitations. These findings are in coherence with those of other researchers (Unal and Zollman, 2000; Petri and Niedderer, 2001; Olsen, 2002; Dimopoulos and Kalkanis, 2005). It seems that 3D visualizations concerning the QAM do not improve students' understanding. The didactic transformation together with the specific learning activities are those that count in combination with them.

On the other hand, it is accepted that it is not possible to combine the graphs of radial and angular wave functions in order to create the representation of an orbital and the corresponding charge density in space (Murell et al., 1985). In other words, it is not possible to visualize the atomic model of a chemical element to support students for the creation of mental images consistent with scientific knowledge and to overcome the difficulties that come from the Bohr model.

In order to overcome these difficulties, we suggest the use of ICT for creating dynamic 3D visualizations of atoms according to Quantum Mechanics principles, following Margel's approach stating that "it is generally accepted that active visualization-based learning can improve understanding and retention, but at the same time interpretation of visual experience highly depends on existing knowledge" (Margel et al., 2004). For the creation of a 3D environment concerning the visualization of the QAM, we have to take into consideration the following remarks:

- to integrate the visualization in a proper educational environment so as to conduct students to comprehend the abstract notions and construct their personal knowledge;
- to explicitly describe the concepts involved in the visualization (e.g. charge density), for students not to keep their misconceptions or construct new ones.

Our intention is to create visualizations of the charge cloud in order to represent the atomic model of hydrogen and picture it in different states.

More specifically, our visualizations will have the following characteristics:

- Give a sense of the 3D space and the spatial distribution of charge clouds, using specific peripheral devices such as stereoscopic glasses.
- Give the possibility to students to freely navigate outside and inside the atom.
- Give the possibility to students to interact and change energy states.
- Give the possibility to students to comprehend the electron's properties.

We believe that the above attributes are implemented using Virtual Reality (VR) technologies and we work to build educational dynamic virtual environments based on scientific data. Virtual Reality has the ability to give substance to abstract concepts and to visualize situations which cannot be seen otherwise and moreover to immerse the student within them (Trindade et al., 2002). So, it seems that VR is a powerful tool for visualizing complex data for helping students to create mental representations that better approach the scientific models. Educational virtual environments visualizing both the microcosm such as the plant cell and megacosm such as our solar system have been developed and evaluated by our group, giving positive learning outcomes (Bakas and Mikropoulos, 2003; Mikropoulos et al., 2003).

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